

Composite Grains: Effects of Porosity and Inclusions on the $10\mu\text{m}$ Silicate Feature

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Abstract

We calculate the absorption efficiency of the composite grains, made up of host silicate spheroids and inclusions of ices/graphites/or voids, in the spectral region $7.0 - 14.0\mu\text{m}$. The absorption efficiencies of the composite spheroidal grains for three axial ratios are computed using the discrete dipole approximation (DDA) as well as using the effective medium approximation & T-Matrix (EMT-Tmatrix) approach. We study the absorption as a function of the volume fraction of the inclusions and porosity. In particular, we study the variation in the $10.0\mu\text{m}$ feature with the volume fraction of the inclusions and porosity. We then calculate the infrared fluxes for these composite grains and compare the model curves with the average observed IRAS-LRS curve, obtained for several circumstellar dust shells around stars. These results on the composite grains show that the wavelength of the peak absorption shifts and the width of the $10.0\mu\text{m}$ feature varies with the variation in the volume fraction of the inclusions. The model curves for composite grains with axial ratios not very large ($\text{AR} \sim 1.3$) and volume fractions of inclusions with $f=0.20$, and dust temperature of about $250\text{-}300^\circ\text{K}$, fit the observed emission curves reasonably well.

1 Introduction

Although, the cosmic dust grains are in general not homogeneous spheres, usually the observed absorption, scattering and extinction data are interpreted using calculations based on Mie theory, which is strictly valid for homogeneous spherical particles. Dust grains ejected from stars are more likely to be non-spherical and inhomogeneous, viz. porous, fluffy and composites of many small grains glued together, due to grain-grain collisions, dust-gas interactions and various other processes. Since there is no exact theory to study the scattering properties of these inhomogeneous grains, there is a need for formulating models of electromagnetic scattering by these grains. Mathis & Whiffen (1989), Mathis (1996), Dwek (1997) and Li & Greenberg (1998) have proposed composite grain models consisting of silicate and amorphous carbon as constituent materials. They have used effective medium approximation (EMT) to calculate the optical constants for composite grains and then used the Mie theory to calculate extinction cross sections for spheres. In EMT the inhomogeneous particle is replaced by a homogeneous one with some 'average effective dielectric function'. The effects related to the fluctuations of the dielectric function within the inhomogeneous structures cannot be treated by this approach of the EMT. Iati et al (2004) have studied optical properties of composite grains as grain aggregates of amorphous carbon and astronomical silicates, using the transition matrix approach. Recently Voshchinnikov et al (2006) and Voshchinnikov & Henning (2008) have studied the effect of grain porosity on interstellar extinction, dust temperature, infrared bands and millimeter opacity. They have used both, the EMT-Mie based calculations and layered sphere model.

Earlier, we have used Discrete Dipole Approximation (DDA) to study the extinction properties of the composite grains (Vaidya et al 2007). For the description on the DDA see Draine (1988). The DDA allows the consideration of irregular shape effects, surface roughness and internal structure within the grain (Wolff et al. 1994, 1998 and Voshchinnikov et al. 2005). For discussion and comparison of DDA and EMT methods, including the limits of the effective medium theory, see Bazell and Dwek (1990), Perrin and Lamy (1990), Perrin

and Sivan (1990), Ossenkopf (1991) and Wolff et al (1994).

The paper has the following sections: In section 2 we give the validity criteria for the DDA and the composite grain models. In section 3 we present and discuss the results of our computations and compare the model curves with the observed IR fluxes obtained by IRAS satellite. The main conclusions of our study are given in section 4.

2 Composite grains and DDA

We use the computer code developed by Dobbie (1999) to generate the composite grain models used in the present study. We have studied composite grain models with a host silicate spheroid containing $N = 9640$, 25896 and 14440 dipoles, each carved out from $32 \times 24 \times 24$, $48 \times 32 \times 32$ and $48 \times 24 \times 24$ dipole sites, respectively; sites outside the spheroid are set to be vacuum (void) and sites inside are assigned to be the host material. It is to be noted that the composite spheroidal grain with $N=9640$ has an axial ratio of 1.33, whereas $N=25896$ has the axial ratio 1.5 and $N=14440$ has the axial ratio 2.0. The volume fractions of the graphite inclusions used are 10%, 20% and 30% (denoted as $f=0.1$, 0.2 and 0.3). Details on the computer code and the corresponding modification to the DDSCAT code (Draine & Flatau 2003) are given in Dobbie (1999), Vaidya et al. (2001, 2007) and Gupta et al. (2006). The modified code outputs a three-dimensional matrix specifying the material type at each dipole site; the sites are either silicate, graphite or vacuum (void). For an illustrative example of a composite spheroidal grain with $N=9640$ dipoles, please see Figure 1 (also Vaidya et al, 2007). There are two validity criteria for DDA (see e.g. Wolff et al. 1994); viz. (i) $|m|kd \leq 1$, where m is the complex refractive index of the material, $k=2\pi/\lambda$ is the wavenumber and d is the lattice dispersion spacing and (ii) d should be small enough (N should be sufficiently large) to describe the shape of the particle satisfactorily. The complex refractive indices for silicates and graphite are obtained from Draine (1985, 1987) and that for ice is from (Irvine & Pollack 1968). For any grain model, the number of dipoles required to obtain a reliable computational result can be estimated using the DDSCAT code (see Vaidya and Gupta 1997

and 1999, Vaidya et al 2001). For the composite grain model, if the host grain has N dipoles, its volume is $N(d)^3$ and if 'a' is the radius of the host grain, $N(d)^3 = 4/3\pi(a)^3$, hence, $N = 4\pi/3(a/d)^3$, and if $|m|kd=1$ and $k=2\pi/\lambda$ the number of dipoles N can be estimated at a given wavelength and the radius of the host grain.

It must be noted here that the composite spheroidal grain models with $N=9640$, 25896 and 14440 have the axial ratio 1.33, 1.5 and 2.0 respectively and if the semi-major axis and semi-minor axis are denoted by $x/2$ and $y/2$ respectively, then $a^3 = (x/2) * (y/2)^2$, where 'a' is the radius of the sphere whose volume is the same as that of a spheroid. In order to study randomly oriented spheroidal grains, it is necessary to get the scattering properties of the composite grains averaged over all of the possible orientations; in the present study we use three values for each of the orientation parameters $(\beta, \theta \& \phi)$, i.e. averaging over 27 orientations, which we find quite adequate (see e.g. Wolff et al 1998).

3 Results and Discussion

3.1 Absorption Efficiency of Composite Spheroidal Grains

Earlier, we had studied the extinction properties of composite spheroidal grains in the spectral region $3.4-0.10\mu\text{m}$ (Vaidya et al 2007). In the present paper, we study the absorption properties of the composite spheroidal grains with three axial ratios, viz. 1.33, 1.5 and 2.0, corresponding to the grain models with $N=9640$, 25896 and 14440 respectively, in the wavelength region $7.0-14.0\mu\text{m}$. The inclusions selected are graphites/ices/or voids.

Figure 2 (a-c) shows the Absorption efficiencies (Q_{abs}) for the composite grains with the host silicate spheroids containing 9640, 25896 and 14440 dipoles, corresponding to axial ratio 1.33, 1.5 and 2.0 respectively with a power law size distribution of a range of grain sizes from $0.005-0.250\mu\text{m}$ in steps of $0.005\mu\text{m}$. The three volume fractions, viz. 10%, 20% and 30%, of ice inclusions are also listed in the top (a) panel.

The effect of the variation of volume fraction of inclusions is clearly seen for all the models. It is to be noted that the wavelength of the peak absorption shifts with the variation in the

volume fraction of inclusions. These absorption curves also show the variation in the width of the absorption feature with the volume fraction of inclusions. All these results indicate that the inhomogeneities within the grains play an important role in modifying the $10\mu\text{m}$ feature. It is also seen in Fig. 2 that the shape of the Q_{abs} curve also varies with the axial ratio, AR of the composite grain, and the absorption peak shifts towards shorter wavelength as the AR increases.

O'Donnell (1994) has investigated the variation of the $10\mu\text{m}$ feature with the grain composition using spheroidal composite grains containing inclusions of either amorphous carbon, tholins or vacuum. He found that the inclusion of tholins or carbon increases the absorption on the short wavelength side of the $10\mu\text{m}$ feature. Further, the inclusion of tholin also broadens the $10\mu\text{m}$ feature.

Figure 3 shows the absorption efficiency for the composite grains ($N=9640$, $AR=1.33$, $a=0.10\mu\text{m}$) with host silicate and graphite inclusions (thick lines). It is seen that the Q_{abs} decreases as the the volume fraction of inclusions ' f ' increases and the absorption peak shifts towards shorter wavelength and broadens with the volume fraction of inclusions. We have compared our results on the absorption efficiencies of the composite grains obtained using the DDA with the results obtained using the EMT-T matrix based calculations. These results are also displayed in Figure 3 (in thin lines). For these calculations, the optical constants were obtained using the Maxwell-Garnet mixing rule (Bohren and Huffman 1983). Description of the T-matrix method/and code is given by Mishchenko (2002).

Since Maxwell-Garnett rule provides the extreme cases of the possible values of the effective dielectric constants of the two-component mixture (see Chylek et al, 2000), we have used this rule. On the other hand, Bruggeman mixing rule applies to a two-component mixture with no distinguishable inclusions embedded in a definite matrix; i.e. it applies to a completely randomly inhomogeneous medium (Bohren & Hoffman, 1983). In the figure 3 we have also shown the absorption efficiency for the composite grain with $f=0.2$ using Bruggeman rule.

It is seen that the absorption curves obtained using EMTs (Maxwell-Garnett and Bruggeman mixing rules) deviate considerably from the curves obtained using DDA. The DDA allows consideration of irregular shape effects, surface roughness and internal structure within the grain (Wolff et al 1994, 1998). In EMT the inhomogeneous grain is replaced by a homogeneous one with some 'average effective dielectric function', the effects related to the fluctuations of the dielectric function within the inhomogeneous structures can not be treated by the EMTs and material interfaces and shapes are smeared out into a homogeneous 'average mixture' Saija et al 2001). Perrin and Lamy (1990) have calculated extinction cross sections for the composite grains, using both the EMTs, as well as the DDA. They found that for small porous grains the results given by Maxwell-Garnett are much better than the results given by the Bruggeman theory. The criteria of validity of the respective effective theories are not clear (Perrin and Lamy, 1990). We have used more accurate DDA method to calculate the absorption cross sections for the composite grains. However, it would still be very useful and desirable to compare the DDA results for the composite grains with those computed by other EMT/Mie type/T matrix techniques in order to examine the applicability of several mixing rules. (see Wolff et al 1998, Voshchinnikov and Mathis 1999, Chylek et al. 2000, Voshchinnikov et al 2005, 2006). The application of DDA, poses a computational challenge, particularly for the large values of the size parameter $X(= 2\pi a/\lambda > 20)$ and the complex refractive index m of the grain material would require large number of dipoles and that in turn would require considerable computer memory and cpu time (see e.g. Saija et al 2001, Voshchinnikov et al 2006).

We have also calculated the absorption efficiencies of the porous silicate grains. Figure 4 shows the absorption efficiencies of the composite grains ($N=9640$) with the host silicate spheroids and voids as inclusions in three volume fractions viz. 0.05, 0.10 and 0.20 for the three grain sizes viz. $a=0.1, 0.2$ and $0.5\mu\text{m}$. These results show that the peak strength decreases with the porosity. It is also seen that the peak of the $10\mu\text{m}$ shifts and broadens as the porosity increases. Voshchinnikov et al (2006) and Voshchinnikov & Henning (2008) have

used layered spheres model combining all components including vacuum, to study the effect of porosity on the $10\mu\text{m}$ feature. Voshchinnikov & Henning (2008) found the peak strength decreases and the feature also broadens with increasing porosity. These results are consistent with the results we have obtained with our composite grain model. Recently, Li et al (2008) have also used the porous grains to model the $9.7\mu\text{m}$ feature in the AGN. They have used multilayered sphere model of Voshchinnikov & Mathis (1999) and calculated the absorption efficiency of porous composite dust consisting amorphous silicate, amorphous carbon and vacuum. Li et al (2008) have found the progressive broadening of the $10\mu\text{m}$ feature and shift to longer wavelengths of the peak position of the feature as the porosity increases.

3.2 Infrared Emission from Circumstellar Dust: Silicate Feature at $9.7\mu\text{m}$

In general, stars which have evolved off the main sequence and which have entered the giant phase of their evolution are a major source of dust grains in the galactic interstellar medium. Such stars have oxygen overabundant relative to carbon and therefore produce silicate dust and show the strong feature at $9.7\mu\text{m}$. This is ascribed to the Si-O stretching mode in some form of silicate material, e.g. olivine. These materials also have a feature at $18\mu\text{m}$, resulting from the O-Si-O bending mode (Evans, 1993).

Using the absorption efficiencies of the composite grains, we calculate the infrared flux, F_λ at various temperatures of the dust, and for a power law MRN dust grain size distribution (Mathis et al 1977). We compare the model curves with the average observed LRS-IRAS curve, obtained for several circumstellar dust shells around stars. Figure 5(a) shows the infrared flux at the dust temperature $T=250^\circ\text{K}$ for the composite grains containing number of dipoles $N=9640$, for three volume fractions of void inclusions (porous). Figure 5(b) shows infrared flux at $T=450^\circ\text{K}$ for the composite grains with voids as inclusions.

Figure 6 shows the variation of infrared flux between $T=200$ and 500°K , for the porous grains. In this figure we have also shown the average observed IRAS-LRS curve (Whittet 2003).

These results show that the composite grains with number of dipoles, $N=9640$ and porosity $f=0.2$, and dust temperature around 300°K fit the observed infrared flux (Whittet, 2003) reasonably well. It is to be noted here that Voshchinnikov & Henning (2008) have compared the results of the porous composite grains with the spectra of T Tauri and Herbig Ae/Be stars, Li et al (2008) have compared the porous grain models with the AGNs, whereas in this paper we have compared the composite grain models with the average observed IRAS flux (Whittet, 2003).

4 Summary and Conclusions

Using the discrete dipole approximation (DDA) we have studied the variation of the absorption efficiency for the composite spheroidal grains, with the volume fractions of the inclusions in the wavelength region of $7.0\text{-}14.0\mu\text{m}$. These results clearly show the variation in the absorption efficiency for the composite grains with the volume fractions of the inclusions. The results on the composite grains also show the shift in the peak absorption wavelength $9.7\mu\text{m}$ with the volume fraction of the inclusions and porosity. The results obtained using DDA based calculations deviate considerably from the results obtained using EMT-TMatrix calculations.

The results on the composite grains clearly show that the inhomogeneity in the grains modifies the absorption/emission properties of the grains. Further study on the emission properties of composite grains at longer wavelengths in the IR is in progress (Vaidya et al 2008).

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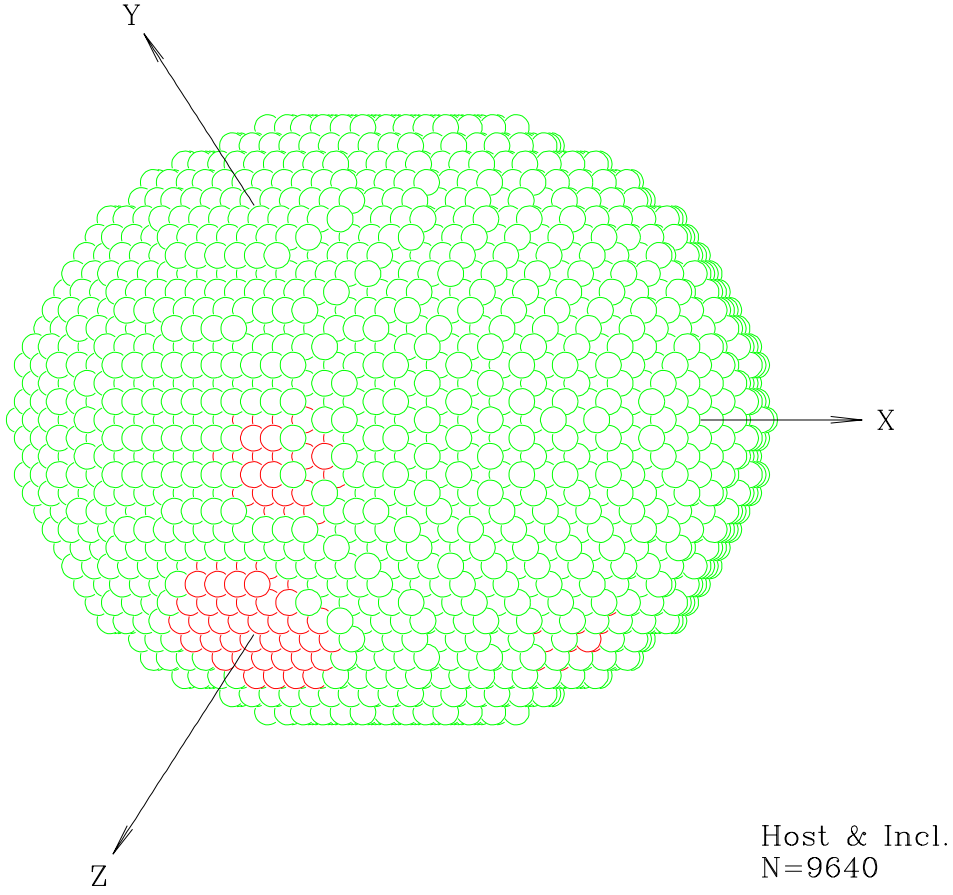


Figure 1: A typical non-spherical composite grain with a total of $N=9640$ dipoles where the inclusions embedded in the host spheroid are shown such that only the ones placed at the outer periphery are seen (Reproduced from Vaidya et al, 2007).

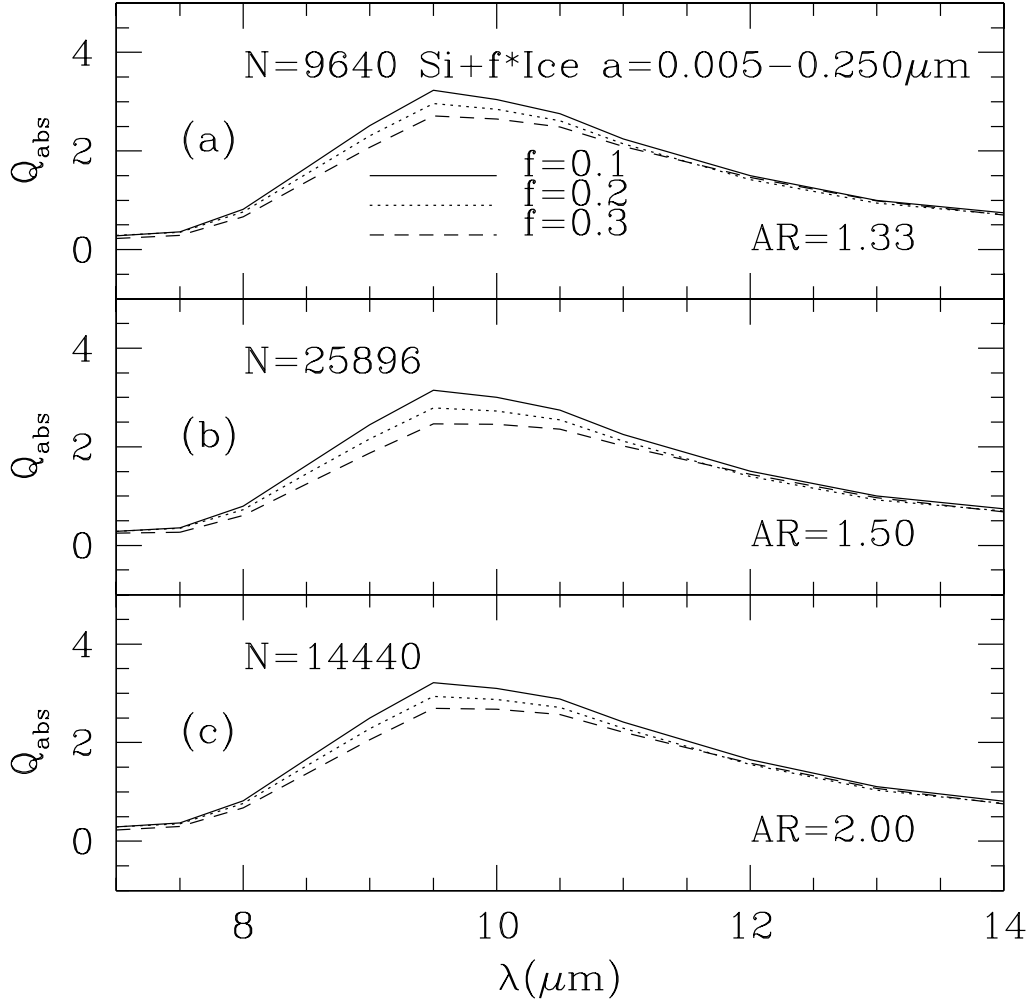


Figure 2: Absorption Efficiencies for the composite grains with host silicate spheroids containing $N=9640$; 25896 & 14440 dipoles and ices as inclusions for three volume fractions.

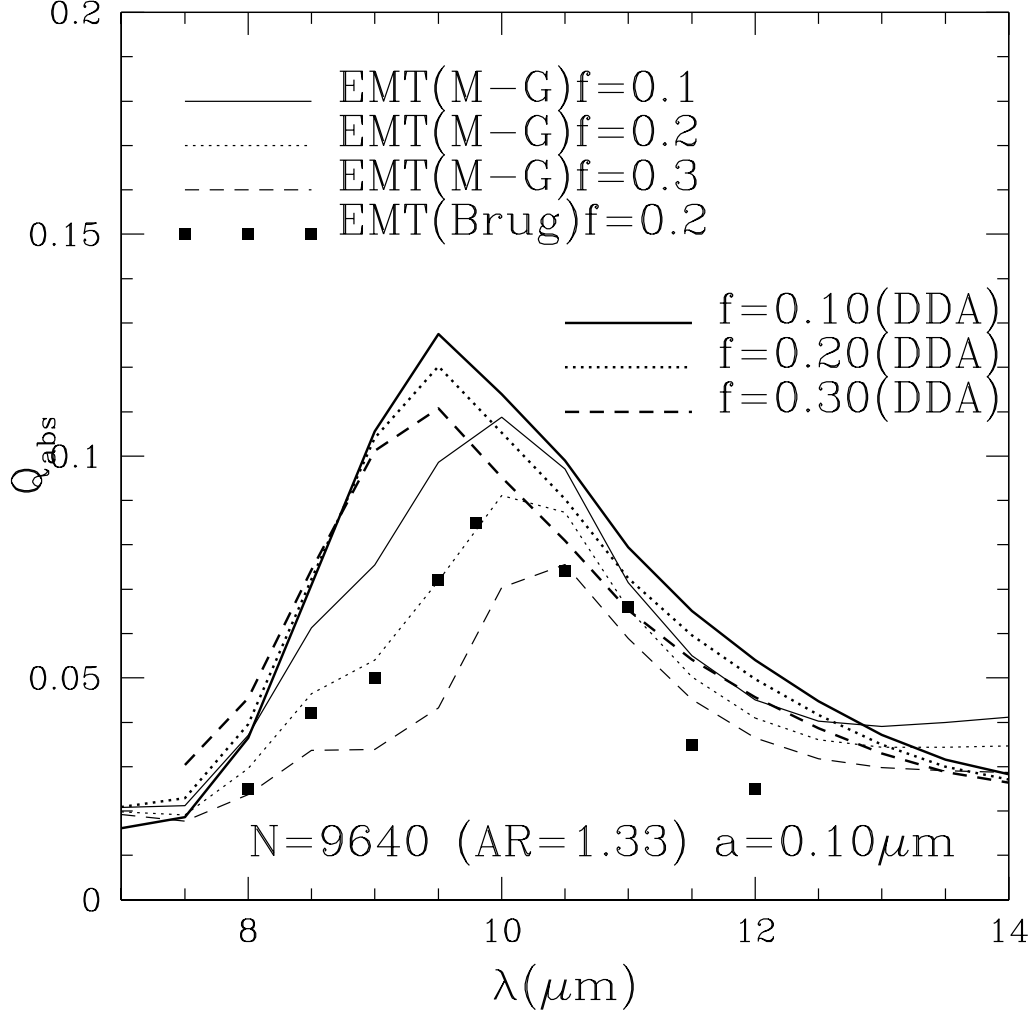


Figure 3: Absorption efficiencies for the composite grains, with host silicate spheroids containing $N=9640$ dipoles and graphite as inclusions for three volume fractions for a grain size of $a=0.10\mu\text{m}$ (thick lines). Also shown are the EMT-T matrix calculations with the same axial ration $AR=1.33$ and three volume fractions (thin lines). The dots represent Bruggeman rule calculations for $f=0.2$.

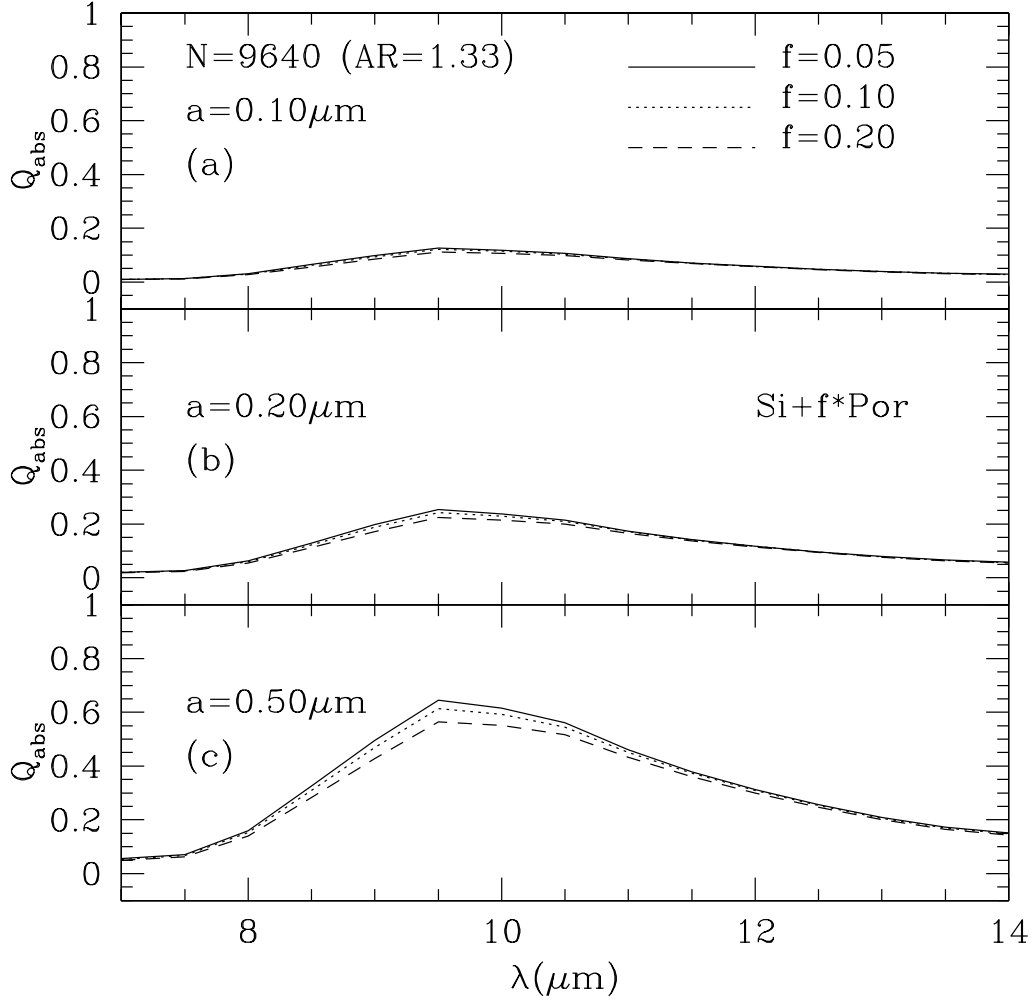


Figure 4: Absorption Efficiencies for the porous silicate grains with $N=9640$, three volume fractions and three grain sizes.

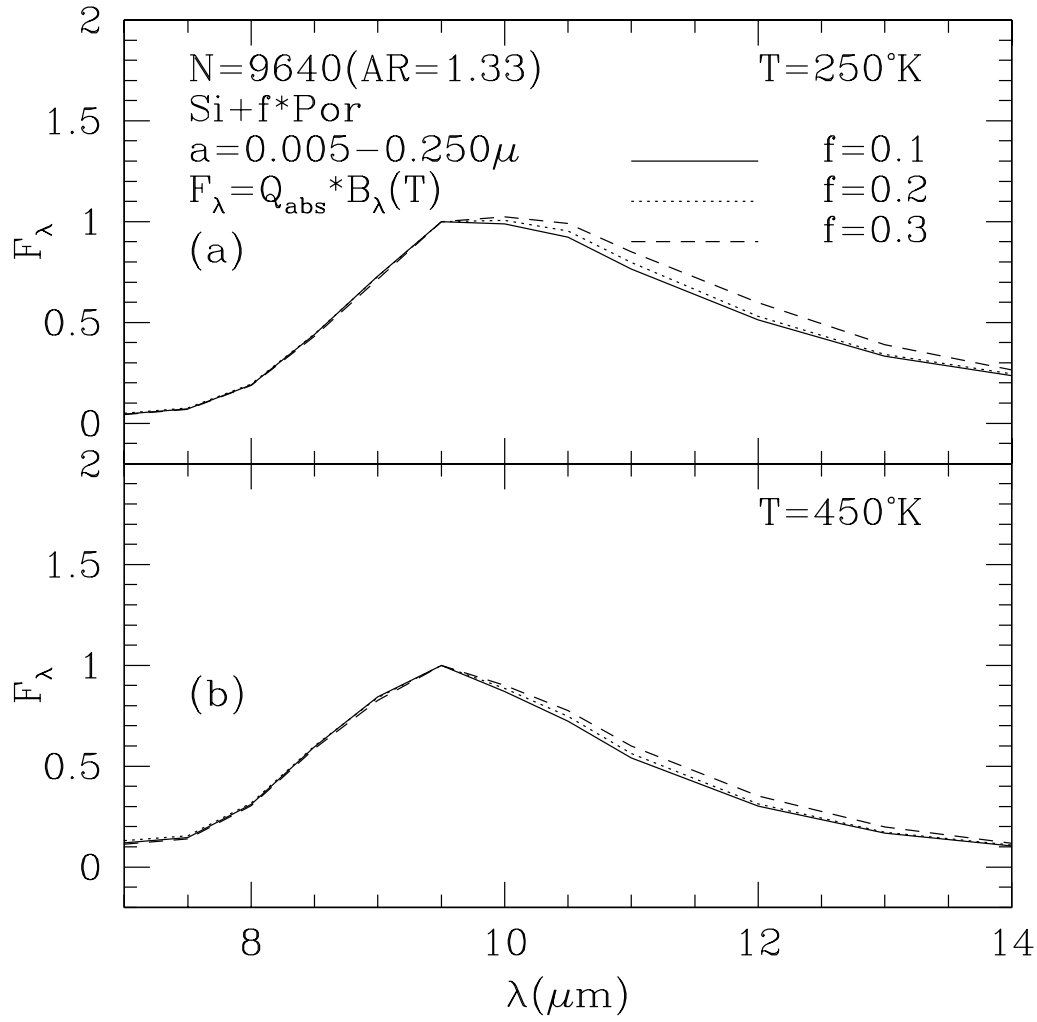


Figure 5: Infrared flux for the composite grains with voids as inclusions (porous), in the wavelength range of 7-14 μm ., at the dust temperatures of $T=250$ & 450°K in panels (a) and (b) respectively.

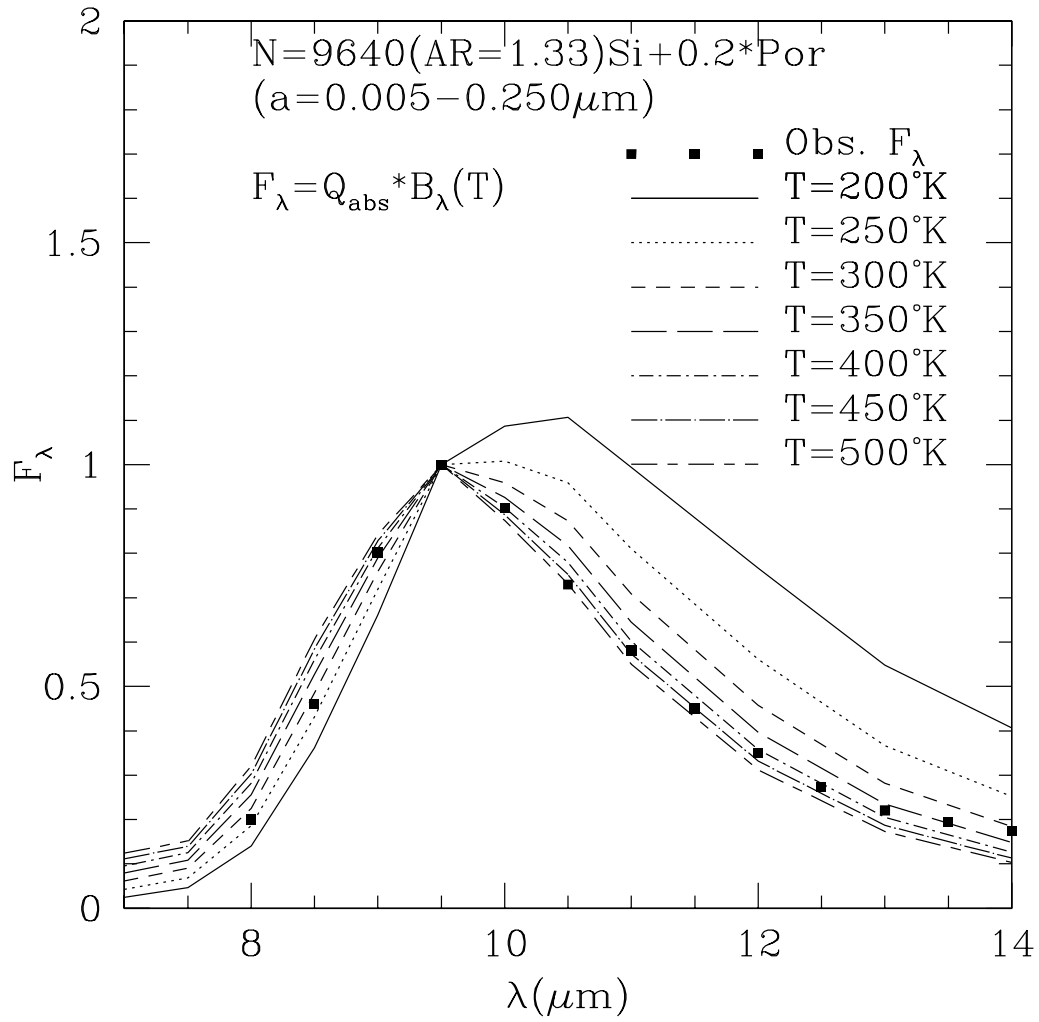


Figure 6: Infrared flux for the composite grains with voids as inclusions at various dust temperatures. The average observed IRAS IR flux values are also shown (in square dots) for comparison.